The Claims:

1. (Currently Amended) An apparatus comprising:

one or more processors; and

a memory coupled to the processors comprising one or more instructions, the processors operable when executing the instructions to:

determine an atom-pair type of a protein-ligand atom pair in a protein-ligand complex;

calculate a repulsion term of the protein-ligand atom pair according to a minimum binding-energy distance value and a well-depth value of the atom-pair type;

calculate a potential of mean force (PMF) of the protein-ligand atom pair according to the calculated repulsion term of the protein-ligand atom pair; ~~and~~

calculate a PMF score of the protein-ligand complex according to the calculated PMF of the protein-ligand atom pair, the PMF score indicating a binding affinity between a protein and a ligand in the protein-ligand ~~complex.~~ complex; and

communicate the PMF score for presentation to a user.

2. (Previously Presented) The apparatus of Claim 1, wherein the minimum binding-energy distance value of the atom-pair type is an empirically derived minimum binding-energy distance value of the atom-pair type and the well-depth value of the atom-pair type is an empirically derived well-depth value of the atom-pair type.

3-4 (Canceled)

5. (Previously Presented) The apparatus of Claim 2, wherein a first set of empirically derived minimum binding-energy distances and well-depth values comprises the minimum binding-energy distance value and the well-depth value of the atom-pair type, the first set yielding a better agreement with a plurality of actual analyzed protein-ligand atom pairs than one or more second sets of empirically derived minimum binding-energy distances and well-depth values.

6. (Canceled)

7. (Previously Presented) The apparatus of Claim 5, wherein root mean square (RMS) deviation between actual analyzed protein-ligand complex structures and protein-ligand complex structures predicted according to a set of empirically derived minimum binding-energy distances and well-depth values determines agreement between the set of empirically derived minimum binding-energy distances and well-depth values and the actual analyzed protein-ligand atom pairs.

8. (Canceled)

9. (Previously Presented) The apparatus of Claim 5, wherein one or more of the first set of empirically derived minimum binding-energy distances and well-depth values or second sets of empirically derived minimum binding-energy distances and well-depth values are each a product of one or more manual processes or automatic processes.

10. (Previously Presented) The apparatus of Claim 9, wherein at least one of the automatic processes comprises execution of a genetic algorithm.

11. (Currently Amended) A method comprising:

determining an atom-pair type of a protein-ligand atom pair in a protein-ligand complex;

calculating a repulsion term of the protein-ligand atom pair according to a minimum binding-energy distance value and a well-depth value of the atom-pair type;

calculating a potential of mean force (PMF) of the protein-ligand atom pair according to the calculated repulsion term of the protein-ligand atom pair; ~~and~~

calculating a PMF score of the protein-ligand complex according to the calculated PMF of the protein-ligand atom pair, the PMF score indicating a binding affinity between a protein and a ligand in the protein-ligand ~~complex.~~ complex; and

communicating the PMF score for presentation to a user.

12. (Previously Presented) The method of Claim 11, wherein the minimum binding-energy distance value of the atom-pair type is an empirically derived minimum binding-energy distance value of the atom-pair type and the well-depth value of the atom-pair type is an empirically derived well-depth value of the atom-pair type.

13-14 (Canceled)

15. (Previously Presented) The method of Claim 12, wherein a first set of empirically derived minimum binding-energy distances and well-depth values comprises the minimum binding-energy distance value and the well-depth value of the atom-pair type, the first set yielding a better agreement with a plurality of actual analyzed protein-ligand atom pairs than one or more second sets of empirically derived minimum binding-energy distances and well-depth values.

16. (Canceled)

17. (Previously Presented) The method of Claim 15, wherein root mean square (RMS) deviation between actual analyzed protein-ligand complex structures and protein-ligand complex structures predicted according to a set of empirically derived minimum binding-energy distances and well-depth values determines agreement between the set of empirically derived minimum binding-energy distances and well-depth values and the actual analyzed protein-ligand atom pairs.

18. (Canceled)

19. (Currently Amended) The method of ~~Claim 5, wherein~~ Claim 15, wherein one or more of the first set of empirically derived minimum binding-energy distances and well-depth values or second sets of empirically derived minimum binding-energy distances and well-depth values are each a product of one or more manual processes or automatic processes.

20. (Previously Presented) The method of Claim 19, wherein at least one of the automatic processes comprises execution of a genetic algorithm.

21. (Currently Amended) ~~Logic encoded in one or more tangible media for execution and~~ Software encoded in one or more computer-readable tangible media and when executed operable to:

determine an atom-pair type of a protein-ligand atom pair in a protein-ligand complex;

calculate a repulsion term of the protein-ligand atom pair according to a minimum binding-energy distance value and a well-depth value of the atom-pair type;

calculate a potential of mean force (PMF) of the protein-ligand atom pair according to the calculated repulsion term of the protein-ligand atom pair; ~~and~~

calculate a PMF score of the protein-ligand complex according to the calculated PMF of the protein-ligand atom pair, the PMF score indicating a binding affinity between a protein and a ligand in the protein-ligand ~~complex.~~ complex; and

communicate the PMF score for presentation to a user.

22. (Currently Amended) The ~~logic~~ software of Claim 21, wherein the minimum binding-energy distance value of the atom-pair type is an empirically derived minimum binding-energy distance value of the atom-pair type and the well-depth value of the atom-pair type is an empirically derived well-depth value of the atom-pair type.

23-24 (Canceled)

25. (Currently Amended) The ~~logic~~ software of Claim 22, wherein a first set of empirically derived minimum binding-energy distances and well-depth values comprises the minimum binding-energy distance value and the well-depth value of the atom-pair type, the first set yielding a better agreement with a plurality of actual analyzed protein-ligand atom pairs than one or more second sets of empirically derived minimum binding-energy distances and well-depth values.

26. (Canceled)

27. (Currently Amended) The ~~logic~~ software of Claim 25, wherein root mean square (RMS) deviation between actual analyzed protein-ligand complex structures and protein-ligand complex structures predicted according to a set of empirically derived minimum binding-energy distances and well-depth values determines agreement between the set of empirically derived minimum binding-energy distances and well-depth values and the actual analyzed protein-ligand atom pairs.

28. (Canceled)

29. (Currently Amended) The ~~logic~~ software of Claim 25, wherein one or more of the first set of empirically derived minimum binding-energy distances and well-depth values or second sets of empirically derived minimum binding-energy distances and well-depth values are each a product of one or more manual processes or automatic processes.

30. (Currently Amended) The ~~logic~~ software of Claim 29, wherein at least one of the automatic processes comprises execution of a genetic algorithm.

31. (Currently Amended) A system comprising:

means for determining an atom-pair type of a protein-ligand atom pair in a protein-ligand complex;

means for calculating a repulsion term of the protein-ligand atom pair according to a minimum binding-energy distance value and a well-depth value of the atom-pair type;

means for calculating a potential of mean force (PMF) of the protein-ligand atom pair according to the calculated repulsion term of the protein-ligand atom pair; ~~and~~

means for calculating a PMF score of the protein-ligand complex according to the calculated PMF of the protein-ligand atom pair, the PMF score indicating a binding affinity between a protein and a ligand in the protein-ligand ~~complex.~~ complex; and

means for communicating the PMF score for presentation to a user.